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Original Research Article

Stability characteristics of single-walled boron nitride nanotubes

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ABSTRACT

Boron nitride nanotubes, like carbon nanotubes, possess extraordinary mechanical properties. Herein, a three-dimensional finite element model is proposed in which the nanotubes are modeled using the principles of structural mechanics. To obtain the properties of this model, a linkage between the molecular mechanics and the density functional theory is constructed. The model is utilized to study the buckling behavior of single-walled boron nitride nanotubes with different geometries and boundary conditions. It is shown that at the same radius, longer nanotubes are less stable. However, for sufficiently long nanotubes the effect of side length decreases.

1. Introduction

The discovery of carbon nanotubes (CNTs) by Iijima [1] attracted a great deal of research community attention. This is mainly due to their unique mechanical, electrical and thermal properties [2–4]. The existence possibility of some non-carbon nanotubes such as boron nitride nanotubes (BNNTs) was also studied by some researchers [5,6]. It has been shown that BNNTs, like CNTs, possess extraordinary mechanical properties, such as high tensile rigidity [7,8], high thermal conductivity along the nanotube [9], and good resistance to oxidation at high temperature [10]. Some experimental studies have been done to obtain Young's modulus of BNNTs. Using a direct force method, Golberg et al. [11] predicted Young's modulus as 0.5 TPa. Suryavanshi et al. [12] utilized the electric-field-induced resonance method and computed Young's modulus as 0.8 TPa. Theoretically, Young's modulus has been predicted to be 1.2 TPa [7,13]. However, unlike carbon nanotubes which depending on chirality and diameter show a metallic, semiconductor or insulator characteristic, BNNTs behave as an insulator for low electric fields. This property is independent of their chirality, diameter and number of walls [6].

Generally, two classes of approaches have been used to study the mechanical behavior of nanotubes: atomistic approaches [14–16] and continuum mechanics approaches [17–19]. Song et al. [20] developed a finite-deformation shell theory for BNNTs from the interatomic potential to account for the effect of bending and curvature. Chowdhury et al. [21] used molecular mechanics simulations and continuum mechanics theories to study the axial, torsional, transverse and radial breathing vibrations of BNNTs. They obtained that the equivalent Young's modulus and shear modulus of BNNTs, independent of the chirality, are 1 TPa and 0.4 TPa, respectively.

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To compute the properties of this model, some force constants should be obtained. On the basis of the electronic structure of molecules calculations, an accurate model is proposed by the quantum mechanics. But, despite of the accuracy, this model is computationally expensive and even with exerting the simplifications it is very time consuming. On the basis of the Born–Oppenheimer approximation, the motion of electrons can be ignored in the molecular mechanics and system energy can be described as a function of nucleus position. Even though the speed of calculation is increased by this simplification, the accuracy decreases. This disadvantage is solved through a linkage between the molecular mechanics and the density functional theory (DFT) in this article. A three dimensional finite element (FE) model, named as space frame model, is used to study the mechanical behavior of single-walled boron nitride nanotubes (SWBNNTs). The DFT calculations are used to obtain accurate force constants which are employed in determining element properties. Based on the model developed, the buckling behavior of SWBNNTs is studied.

2. Molecular mechanics modeling

Based on the molecular mechanics, the total potential energy can be expressed by the summation of several energies due to bonded interactions or bonded and non-bonded interactions [22,23]

$$E_t = U_\rho + U_\theta + U_\omega + U_\tau + U_{vdw} + U_{es} \tag{1}$$

in which U_ρ, U_θ, U_ω, and U_τ are energies associated with bond stretching, bond angle variation, bond inversion, and torsion, respectively; U_{vdw} and U_{es} are also associated with van der Waals and electrostatic interactions respectively.

These energy terms can be explained in different energy functions with respect to the material and loading conditions. For single-walled nanotubes, it can be expected that U_ρ, U_θ, and U_ω are the main components of the total potential energy and also U_{vdw} can be omitted. In small deformations conditions, Hooke law is assessed to be such an accurate and efficient enough to be used for describing the interaction between atoms in the system. Accordingly Eq. (1) can be written as the following form

$$E_t = \sum \frac{1}{2} K_\rho (\Delta r)^2 + \sum \frac{1}{2} C_\theta (\Delta\theta)^2 + \sum \frac{1}{2} C_\omega (\Delta\phi)^2 \tag{2}$$

in which Δr, $\Delta\theta$ and $\Delta\phi$ are the bond elongation, bond angle variance and the change of space between two atoms, respectively. Force constants of K_ρ, C_θ and C_ω are related to the stretching energy due to bond link variation, bond angle variation and bond torsion, respectively (see Fig. 1.), and they can be calculated theoretically or experimentally.

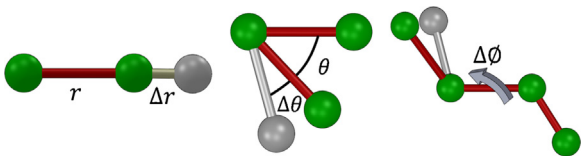

Fig. 1 – Different bonds structure of a BN cell corresponding to each energy term.

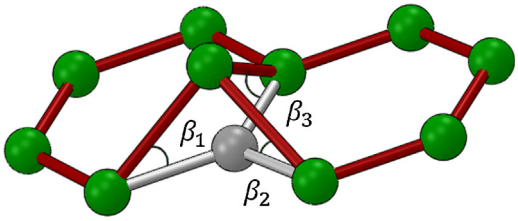

Fig. 2 – The components of average inversion angle ∅.

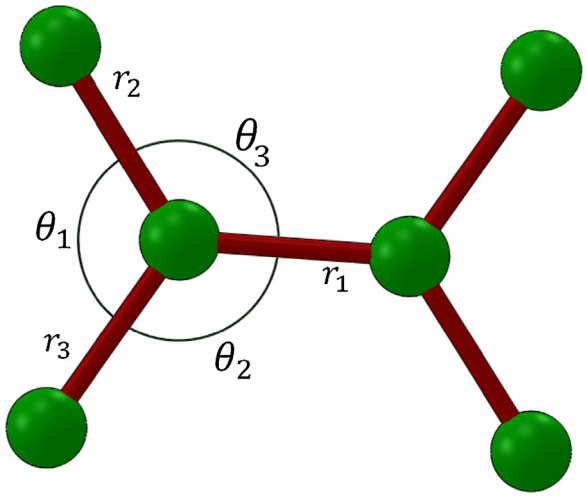

Fig. 3 – Definition for atom position of type A and B in a chiral tube.

The average inversion angle ϕ can be computed as

$$\phi = \frac{1}{3}(\beta_1 + \beta_2 + \beta_3) \tag{3}$$

The angles β_1, β_2 and β_3 have been represented in Fig. 2.

As it has been represented in Fig. 3, because of three bond length and three bond angles associated with an atom with ij indexes in a nanotube, Eq. (2) can be written in another form as follows

$$E_t = \frac{1}{2}\sum_{ij}\frac{1}{2}K_\rho \sum_k (dr_{ijk})^2 + \sum_{ij}\frac{1}{2}C_\theta \sum_k (d\theta_{ijk})^2 + \sum_{ij}\frac{1}{2}C_\omega \left(\frac{1}{3}\sum_k d\beta_{ijk}\right)^2 \quad k = 1,2,3 \tag{4}$$

in which the coefficient 1/2 in the first term of Eq. (4) implies that the bond stretching energy is accounted only once.

The axial force of F acting on the chiral single-walled nanotubes can be decomposed into two components of f_p and f_a which are respectively perpendicular to the bond of r_3 and along it (see Fig. 4).

Geometric relationship between these two forces is as follows

$$f_p = F\cos\left(\frac{\pi}{6} - \Theta\right) \tag{5}$$

$$f_a = F\sin\left(\frac{\pi}{6} - \Theta\right) \tag{6}$$